Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,2′-[1,1′-(Propane-2,2-diyldiimino)-diethylidene]diphenol

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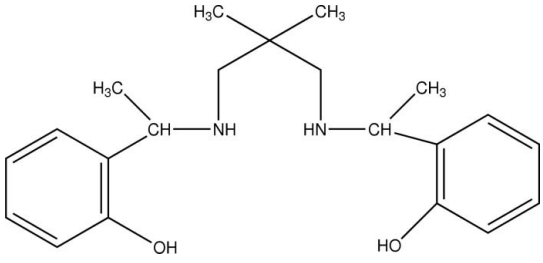
Received 6 August 2007; accepted 8 August 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.061; wR factor = 0.207; data-to-parameter ratio = 25.9.

In the crystal structure of the title compound, $C_{21}H_{30}N_2O_2$, intermolecular N—H···O hydrogen bonds result in the formation of chains along the b axis. Intramolecular O—H···N and N—H···O hydrogen bonds are also present.

Related literature

For general backgroud, see: Burgess *et al.* (1999); Höpfl *et al.* (1998); Maciejewska *et al.* (1999); Mitra *et al.* (2004, 2006); Yalçın *et al.* (2001). For bond-length data, see: Allen *et al.* (1987); Sanchez *et al.* (2004).



Experimental

Crystal data

$C_{21}H_{30}N_2O_2$
M_r = 342.47
Monoclinic, $P2_1/c$
a = 11.4232 (3) Å
b = 10.1303 (3) Å
c = 18.4399 (4) Å
β = 107.753 (5)°
V = 2032.26 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 298 (2) K
0.2 × 0.13 × 0.1 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.986, T_{max} = 0.986
57575 measured reflections
6244 independent reflections
3287 reflections with $I > 2\sigma(I)$
R_{int} = 0.063

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.207
S = 1.03
6244 reflections
241 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O2	0.85 (2)	2.53 (2)	3.254 (2)	144.9 (15)
O1—H1O···N1	0.82	1.92	2.648 (2)	147
N2—H2N···O1^{i}	0.95 (2)	2.49 (2)	3.3833 (19)	155.1 (19)
O2—H2O···N2	0.82	1.95	2.671 (2)	147

Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors are indebted to the Department of Chemistry, Atatürk University, Turkey, for the use of the X-ray diffractometer purchased under grant No. 2003/219 of the University Research Fund.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2308).

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  doi:10.1107/S1600536807039153

supplementary materials

Acta Cryst. (2007). E**63**, o3770 [**doi:10.1107/S1600536807039153**]

2,2'-[1,1'-(Propane-2,2-diyldiimino)diethylidene]diphenol

E. Sahin, R. Bilgiç, A. Kenar and O. Atakol

Comment

It has been reported by many studies that Schiff bases form mononuclear or dinuclear compounds with phenylboronic and boric acids (Burgess *et al.*, 1999; Höpfl *et al.*, 1998; Maciejewska *et al.*, 1999; Mitra *et al.*, 2006; Mitra *et al.*, 2004). In these studies, the compounds of reduced forms of Schiff bases also exist (Mitra *et al.*, 2006). It has been noted that tri- and tetracoordinated compounds are formed between reduced Schiff bases and organic esters of boric acid. In this study, an ONNO type Schiff base has reduced to phenol imine form with the usage of $NaBH_4$ in MeOH media. In fact, it was aimed to prepare a new complex from reaction of Schiff base and phenylboronic acid, but Schiff base crystal which is suitable for X-ray analysis was obtained. When ligand is crystallized in the common solvents, the appropriate single crystals for X-ray analysis could not be obtained. It was concluded that first phenylboronic acid and ligand are formed an intermediate complex, which is affected the solubility of Schiff base. Hence it was inferred that this procedure could be a new recrystallization method for organic ligands. We report herein the crystal structure of the title compound, (I).

In the molecule of (I) (Fig. 1), the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987). In the form of the Schiff base, C=N double bond is about 1.27–1.30 Å (Sanchez *et al.*, 2004). After the reduction reaction of double bond, it was converted to mono bonds (C7—N1 [1.483 (2) Å] and C13—N2 [1.481 (2) Å]). The strong hydrogen bond between iminic nitrogen (in the form of Schiff base) and phenol group continued after reduction (Yalçın *et al.*, 2001).

Rings A (C1—C6) and B (C15—C20) are, of course, planar and the dihedral angle between them is A/B = 89.65 (2)°.

In the crystal structure, intermolecular N—H···O and intramolecular O—H—N and N—H—O hydrogen bonds (Table 1) result in the formation of chains along the *b* axis (Fig. 2), in which they seem to be effective in the stabilization of the structure.

Experimental

The ligand was prepared in two steps. In the first step, the Schiff base was synthesized from 2-hydroxy acetophenone (2.72 g. 20 mmol) and 2,2'-dimethyl −1,3-propanediamine (1.02 g, 10 mmol) in MeOH (50 ml) solution. The mixture was heated until boiling temperature and left to stand on air. After one day, the yellow Schiff base was crystallized. In the second step, the Schiff base (2.0 g) was dissolved in hot MeOH (100 ml) and a piece of solid $NaBH_4$ was added slowly to this solution until it turned colorless. The reduced Schiff base precipitated after addition of ice. The mixture was left to stand at 277 K for 1 d to obtain crystals, and then was filtered. The crystals were allowed to dry on air. For the preparation of the title complex, the ligand (0.689 g, 2 mmol) was dissolved in hot MeOH (50 ml) and the solution of phenylboronic acid (0.244 g, 2 mmol) in hot acetonitrile (40 ml.) was added. The colorless crystals of (I) were obtained by filtration after 2 d and allowed to dry on air.

Refinement

H1N and H2N (for NH_2) were located in difference syntheses and refined isotropically [N—H = 0.846 (19) and 0.95 (2) Å, U_{iso}(H) = 0.064 (5) and 0.091 (7) Å^2]. The remaining H atoms were positioned geometrically, with O—H = 0.82 Å (for OH), C—H = 0.93, 0.98, 0.97 and 0.96 Å for aromatic, methine, methylene and methyl H, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C,O)$, where x = 1.2 for aromatic, methine and methylene H, and x = 1.5 for all other H atoms.

Figures

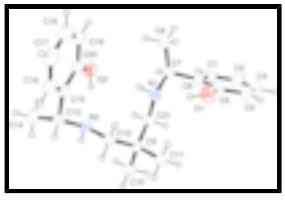


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

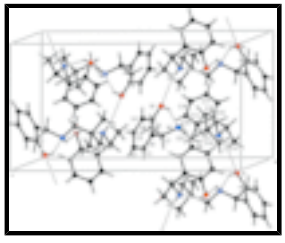


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

2,2'-[1,1'-(Propane-2,2-diyldiimino)diethylidene]diphenol

Crystal data

$C_{21}H_{30}N_2O_2$	F_{000} = 744
M_r = 342.47	D_x = 1.119 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5943 reflections
a = 11.4232 (3) Å	θ = 2.3–30.5º
b = 10.1303 (3) Å	μ = 0.07 mm^{-1}
c = 18.4399 (4) Å	T = 298 (2) K
β = 107.753 (5)º	Needle, colorless
V = 2032.26 (11) Å^3	0.2 × 0.13 × 0.1 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID-S diffractometer	R_{int} = 0.063
dtprofit.ref scans	θ_{max} = 30.9º
Absorption correction: multi-scan (Blessing, 1995)	θ_{min} = 2.3º
T_{min} = 0.986, T_{max} = 0.986	h = −16→16

57575 measured reflections
6244 independent reflections
3287 reflections with $I > 2\sigma(I)$

$k = -14 \rightarrow 12$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.061$

$wR(F^2) = 0.207$

$S = 1.04$

6244 reflections

241 parameters

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0883P)^2 + 0.1285P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.19$ e Å^{-3}

$\Delta\rho_{min} = -0.15$ e Å^{-3}

Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.016 (3)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.65507 (14)	0.05781 (12)	0.93601 (8)	0.0828 (4)
H1O	0.6018	0.0768	0.8962	0.124*
O2	0.20908 (13)	0.27291 (14)	0.74075 (8)	0.0812 (4)
H2O	0.2582	0.2978	0.7192	0.122*
N1	0.49252 (14)	0.21069 (13)	0.83918 (7)	0.0574 (3)
H1N	0.4199 (18)	0.1886 (17)	0.8146 (10)	0.064 (5)*
N2	0.34204 (12)	0.25810 (14)	0.64438 (8)	0.0575 (3)
H2N	0.361 (2)	0.329 (2)	0.6160 (12)	0.091 (7)*
C1	0.65405 (19)	0.3908 (2)	1.01181 (10)	0.0720 (5)
H1	0.6049	0.4659	1.0031	0.086*
C2	0.7652 (2)	0.3934 (3)	1.06795 (12)	0.0892 (7)
H2	0.7908	0.4689	1.0972	0.107*
C3	0.8377 (2)	0.2830 (3)	1.08019 (12)	0.0967 (8)
H3	0.9127	0.2833	1.1186	0.116*
C4	0.80105 (19)	0.1706 (3)	1.03618 (12)	0.0880 (6)
H4	0.8516	0.0966	1.0447	0.106*
C5	0.68921 (17)	0.16917 (19)	0.97972 (10)	0.0679 (5)
C6	0.61266 (15)	0.27926 (17)	0.96746 (9)	0.0591 (4)
C7	0.48655 (16)	0.27559 (17)	0.91006 (9)	0.0618 (4)
H7	0.4574	0.3664	0.8981	0.074*
C8	0.39556 (19)	0.2018 (2)	0.94084 (12)	0.0862 (6)

H8A	0.3158	0.2028	0.9035	0.129*
H8B	0.3912	0.2439	0.9866	0.129*
H8C	0.4224	0.1121	0.9518	0.129*
C9	0.56465 (14)	0.23663 (14)	0.72343 (9)	0.0519 (4)
C10	0.60725 (17)	0.34573 (17)	0.67959 (10)	0.0658 (4)
H10A	0.5446	0.4122	0.6642	0.099*
H10B	0.6222	0.3086	0.6353	0.099*
H10C	0.6816	0.3847	0.7118	0.099*
C11	0.66557 (16)	0.13156 (17)	0.74808 (10)	0.0661 (4)
H11A	0.7405	0.1719	0.7785	0.099*
H11B	0.6785	0.0922	0.7038	0.099*
H11C	0.6409	0.0648	0.7774	0.099*
C12	0.44819 (14)	0.17011 (15)	0.67180 (9)	0.0550 (4)
H12A	0.4668	0.1326	0.6282	0.066*
H12B	0.426	0.0979	0.6996	0.066*
C13	0.23218 (15)	0.18842 (18)	0.59568 (10)	0.0641 (4)
H13	0.2578	0.1299	0.561	0.077*
C14	0.14172 (19)	0.2887 (2)	0.54867 (12)	0.0884 (6)
H14A	0.1159	0.3468	0.582	0.133*
H14B	0.0715	0.2435	0.5159	0.133*
H14C	0.1806	0.3391	0.5184	0.133*
C15	0.17410 (15)	0.10502 (18)	0.64405 (10)	0.0632 (4)
C16	0.12464 (17)	−0.0173 (2)	0.61865 (13)	0.0813 (6)
H16	0.1345	−0.0517	0.5741	0.098*
C17	0.0609 (2)	−0.0898 (3)	0.65776 (16)	0.0990 (8)
H17	0.0277	−0.1715	0.6396	0.119*
C18	0.0474 (2)	−0.0394 (3)	0.72403 (17)	0.1016 (8)
H18	0.0038	−0.087	0.7505	0.122*
C19	0.09767 (19)	0.0807 (3)	0.75152 (12)	0.0875 (6)
H19	0.089	0.1134	0.7967	0.105*
C20	0.16146 (16)	0.1535 (2)	0.71185 (11)	0.0691 (5)
C21	0.54208 (16)	0.30049 (15)	0.79304 (9)	0.0555 (4)
H21A	0.619	0.3368	0.8251	0.067*
H21B	0.4852	0.3733	0.776	0.067*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0960 (11)	0.0667 (8)	0.0763 (9)	0.0131 (7)	0.0124 (7)	−0.0003 (6)
O2	0.0779 (9)	0.0896 (10)	0.0826 (9)	0.0055 (7)	0.0342 (7)	−0.0072 (7)
N1	0.0613 (9)	0.0585 (8)	0.0518 (7)	−0.0081 (6)	0.0166 (6)	−0.0042 (6)
N2	0.0516 (7)	0.0576 (8)	0.0621 (8)	−0.0012 (6)	0.0154 (6)	0.0016 (6)
C1	0.0836 (13)	0.0765 (12)	0.0631 (10)	−0.0157 (10)	0.0333 (9)	−0.0123 (9)
C2	0.0855 (15)	0.1143 (18)	0.0714 (12)	−0.0345 (14)	0.0292 (11)	−0.0239 (12)
C3	0.0632 (12)	0.153 (2)	0.0696 (12)	−0.0242 (14)	0.0133 (10)	−0.0096 (14)
C4	0.0650 (12)	0.1197 (18)	0.0743 (12)	0.0107 (12)	0.0136 (10)	0.0034 (12)
C5	0.0672 (11)	0.0762 (11)	0.0596 (9)	−0.0021 (9)	0.0185 (8)	−0.0016 (8)
C6	0.0619 (9)	0.0672 (10)	0.0515 (8)	−0.0046 (8)	0.0222 (7)	−0.0038 (7)

C7	0.0648 (10)	0.0678 (10)	0.0555 (9)	0.0005 (8)	0.0223 (8)	−0.0035 (7)
C8	0.0695 (12)	0.1258 (18)	0.0692 (11)	−0.0129 (12)	0.0297 (10)	−0.0042 (11)
C9	0.0525 (8)	0.0499 (8)	0.0542 (8)	−0.0012 (6)	0.0175 (6)	−0.0008 (6)
C10	0.0642 (10)	0.0676 (10)	0.0680 (10)	−0.0069 (8)	0.0239 (8)	0.0051 (8)
C11	0.0620 (10)	0.0659 (10)	0.0699 (10)	0.0075 (8)	0.0192 (8)	−0.0002 (8)
C12	0.0568 (9)	0.0522 (8)	0.0566 (8)	0.0005 (7)	0.0179 (7)	−0.0043 (7)
C13	0.0528 (9)	0.0762 (11)	0.0615 (9)	−0.0068 (8)	0.0148 (7)	−0.0012 (8)
C14	0.0641 (11)	0.1088 (16)	0.0826 (13)	−0.0033 (11)	0.0081 (10)	0.0301 (12)
C15	0.0496 (8)	0.0690 (10)	0.0691 (10)	0.0006 (7)	0.0154 (7)	0.0088 (8)
C16	0.0647 (11)	0.0791 (13)	0.0945 (14)	−0.0097 (10)	0.0160 (10)	0.0026 (11)
C17	0.0769 (14)	0.0833 (15)	0.127 (2)	−0.0152 (11)	0.0160 (14)	0.0230 (14)
C18	0.0696 (13)	0.117 (2)	0.1165 (19)	−0.0062 (13)	0.0258 (13)	0.0496 (16)
C19	0.0674 (12)	0.1145 (17)	0.0850 (13)	0.0118 (12)	0.0297 (10)	0.0290 (13)
C20	0.0537 (9)	0.0791 (12)	0.0752 (11)	0.0087 (8)	0.0204 (8)	0.0151 (9)
C21	0.0601 (9)	0.0494 (8)	0.0556 (8)	−0.0038 (7)	0.0157 (7)	−0.0022 (6)

Geometric parameters (Å, °)

O1—C5	1.372 (2)	C9—C10	1.534 (2)
O1—H1O	0.82	C10—H10A	0.96
O2—C20	1.366 (2)	C10—H10B	0.96
O2—H2O	0.82	C10—H10C	0.96
N1—C21	1.472 (2)	C11—H11A	0.96
N1—C7	1.483 (2)	C11—H11B	0.96
N1—H1N	0.846 (19)	C11—H11C	0.96
N2—C12	1.465 (2)	C12—C9	1.536 (2)
N2—C13	1.481 (2)	C12—H12A	0.97
N2—H2N	0.95 (2)	C12—H12B	0.97
C1—C2	1.372 (3)	C13—C14	1.518 (3)
C1—H1	0.93	C13—H13	0.98
C2—H2	0.93	C14—H14A	0.96
C3—C2	1.370 (4)	C14—H14B	0.96
C3—C4	1.386 (3)	C14—H14C	0.96
C3—H3	0.93	C15—C16	1.383 (3)
C4—H4	0.93	C15—C20	1.391 (3)
C5—C4	1.380 (3)	C15—C13	1.520 (2)
C6—C1	1.390 (2)	C16—H16	0.93
C6—C5	1.392 (3)	C17—C18	1.376 (4)
C6—C7	1.506 (2)	C17—C16	1.382 (3)
C7—C8	1.524 (3)	C17—H17	0.93
C7—H7	0.98	C18—H18	0.93
C8—H8A	0.96	C19—C18	1.375 (4)
C8—H8B	0.96	C19—H19	0.93
C8—H8C	0.96	C20—C19	1.391 (3)
C9—C21	1.528 (2)	C21—H21A	0.97
C9—C11	1.533 (2)	C21—H21B	0.97
C5—O1—H1O	109.5	H10B—C10—H10C	109.5
C20—O2—H2O	109.5	C9—C11—H11A	109.5
C21—N1—C7	111.39 (13)	C9—C11—H11B	109.5

C21—N1—H1N	109.9 (12)	H11A—C11—H11B	109.5
C7—N1—H1N	106.8 (12)	C9—C11—H11C	109.5
C12—N2—C13	112.24 (14)	H11A—C11—H11C	109.5
C12—N2—H2N	110.3 (13)	H11B—C11—H11C	109.5
C13—N2—H2N	108.4 (13)	N2—C12—C9	114.61 (13)
C2—C1—C6	122.0 (2)	N2—C12—H12A	108.6
C2—C1—H1	119	C9—C12—H12A	108.6
C6—C1—H1	119	N2—C12—H12B	108.6
C3—C2—C1	118.9 (2)	C9—C12—H12B	108.6
C3—C2—H2	120.6	H12A—C12—H12B	107.6
C1—C2—H2	120.6	N2—C13—C14	109.33 (16)
C2—C3—C4	121.0 (2)	N2—C13—C15	110.49 (14)
C2—C3—H3	119.5	C14—C13—C15	111.35 (15)
C4—C3—H3	119.5	N2—C13—H13	108.5
C5—C4—C3	119.7 (2)	C14—C13—H13	108.5
C5—C4—H4	120.1	C15—C13—H13	108.5
C3—C4—H4	120.1	C13—C14—H14A	109.5
O1—C5—C4	118.94 (18)	C13—C14—H14B	109.5
O1—C5—C6	120.74 (16)	H14A—C14—H14B	109.5
C4—C5—C6	120.31 (18)	C13—C14—H14C	109.5
C1—C6—C5	118.12 (17)	H14A—C14—H14C	109.5
C1—C6—C7	120.96 (16)	H14B—C14—H14C	109.5
C5—C6—C7	120.88 (15)	C16—C15—C20	118.47 (18)
N1—C7—C6	109.83 (14)	C16—C15—C13	120.38 (17)
N1—C7—C8	109.31 (15)	C20—C15—C13	120.99 (16)
C6—C7—C8	111.43 (14)	C17—C16—C15	121.7 (2)
N1—C7—H7	108.7	C17—C16—H16	119.2
C6—C7—H7	108.7	C15—C16—H16	119.2
C8—C7—H7	108.7	C18—C17—C16	119.1 (2)
C7—C8—H8A	109.5	C18—C17—H17	120.5
C7—C8—H8B	109.5	C16—C17—H17	120.5
H8A—C8—H8B	109.5	C19—C18—C17	120.6 (2)
C7—C8—H8C	109.5	C19—C18—H18	119.7
H8A—C8—H8C	109.5	C17—C18—H18	119.7
H8B—C8—H8C	109.5	C18—C19—C20	120.1 (2)
C21—C9—C11	110.45 (13)	C18—C19—H19	119.9
C21—C9—C10	107.44 (13)	C20—C19—H19	119.9
C11—C9—C10	109.02 (14)	O2—C20—C19	118.30 (19)
C21—C9—C12	111.75 (13)	O2—C20—C15	121.65 (16)
C11—C9—C12	108.07 (13)	C19—C20—C15	120.0 (2)
C10—C9—C12	110.09 (13)	N1—C21—C9	114.66 (12)
C9—C10—H10A	109.5	N1—C21—H21A	108.6
C9—C10—H10B	109.5	C9—C21—H21A	108.6
H10A—C10—H10B	109.5	N1—C21—H21B	108.6
C9—C10—H10C	109.5	C9—C21—H21B	108.6
H10A—C10—H10C	109.5	H21A—C21—H21B	107.6
C21—N1—C7—C6	−77.69 (17)	C11—C9—C21—N1	−65.04 (18)
C21—N1—C7—C8	159.77 (15)	C10—C9—C21—N1	176.16 (13)
C7—N1—C21—C9	173.51 (13)	C12—C9—C21—N1	55.30 (18)

C13—N2—C12—C9	−179.33 (13)	N2—C12—C9—C21	57.33 (17)
C12—N2—C13—C14	−161.12 (15)	N2—C12—C9—C11	179.05 (13)
C12—N2—C13—C15	76.00 (17)	N2—C12—C9—C10	−61.98 (17)
C6—C1—C2—C3	0.5 (3)	C16—C15—C13—N2	−142.22 (16)
C2—C3—C4—C5	−0.7 (3)	C20—C15—C13—N2	42.5 (2)
C4—C3—C2—C1	0.9 (3)	C16—C15—C13—C14	96.1 (2)
O1—C5—C4—C3	179.13 (19)	C20—C15—C13—C14	−79.2 (2)
C6—C5—C4—C3	−0.8 (3)	C20—C15—C16—C17	1.7 (3)
C5—C6—C1—C2	−2.0 (3)	C13—C15—C16—C17	−173.71 (18)
C7—C6—C1—C2	175.56 (16)	C16—C15—C20—O2	179.33 (17)
C1—C6—C5—O1	−177.83 (16)	C13—C15—C20—O2	−5.3 (3)
C7—C6—C5—O1	4.7 (2)	C16—C15—C20—C19	−1.5 (3)
C1—C6—C5—C4	2.1 (3)	C13—C15—C20—C19	173.86 (16)
C7—C6—C5—C4	−175.45 (17)	C16—C17—C18—C19	−0.7 (3)
C1—C6—C7—N1	138.62 (16)	C18—C17—C16—C15	−0.6 (3)
C5—C6—C7—N1	−43.9 (2)	C20—C19—C18—C17	0.9 (3)
C1—C6—C7—C8	−100.1 (2)	O2—C20—C19—C18	179.43 (18)
C5—C6—C7—C8	77.3 (2)	C15—C20—C19—C18	0.3 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···O2	0.85 (2)	2.53 (2)	3.254 (2)	144.9 (15)
O1—H1O···N1	0.82	1.92	2.648 (2)	147
N2—H2N···O1^{i}	0.95 (2)	2.49 (2)	3.3833 (19)	156.00
O2—H2O···N2	0.82	1.95	2.671 (2)	147

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2.

Fig. 1

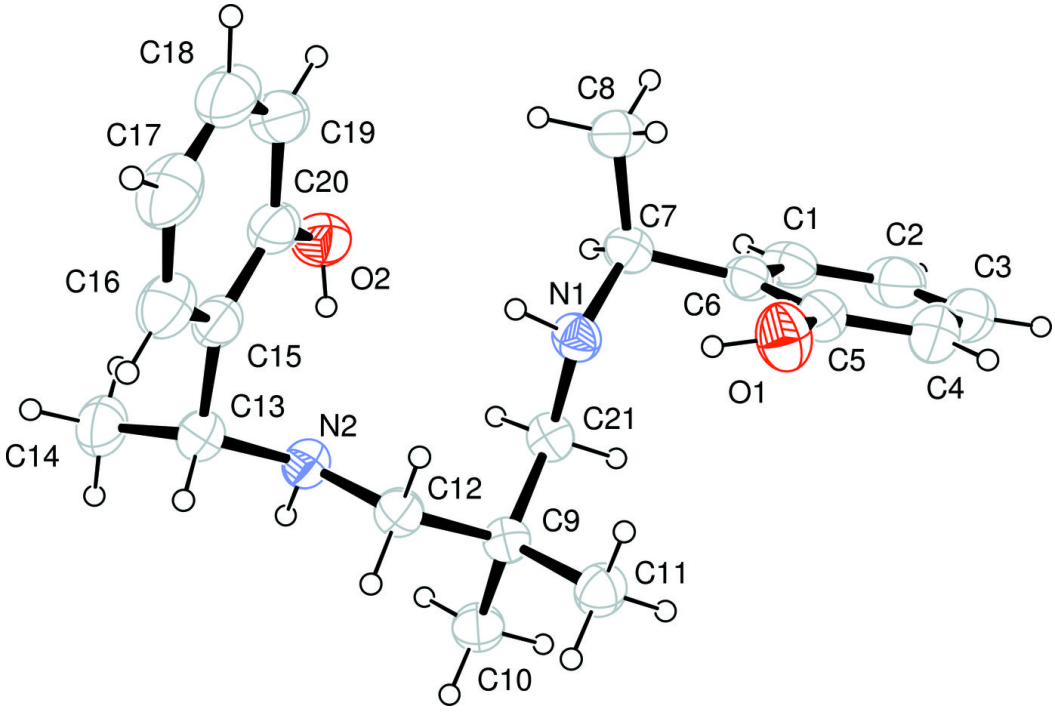
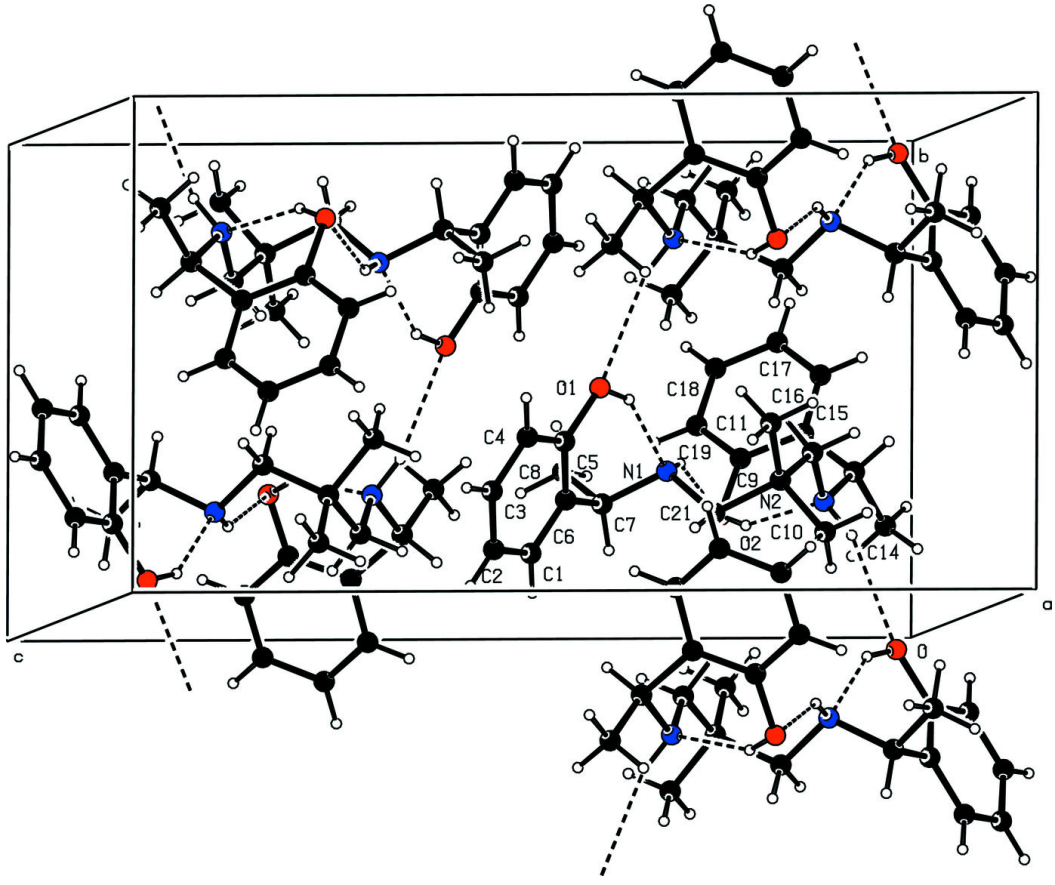

C18
C17
C19
C20
O2
C16
C15
C13
C14
N2
C12
C9
C11
C10
C8
C7
C1
C2
C3
N1
C6
O1
C5
C4
C21

Fig. 2


b
c
a
O1
C4
C8
C5
N1
C3
C6
C7
C2
C1
C18
C17
C16
C15
C11
C19
C9
N2
C21
O2
C10
C14
O